Density Functional Theory and Materials Science: the cases of alloys and carbides

Alfredo Juan

Departamento de Fisica & IFISUR (UNS-CONICET)

Av. Alem 1253, 8000 Bahia Blanca, Argentina

Alloys, intermetallic compounds and transition metal carbides are widely used as catalysts. These are complex materials and about 20% of manufacturing in the industrialized world is dependent on catalysis. Most catalysts used in industry are solids, and the catalysis takes place on the surface of nanoparticles of the active material or in the particle/support interface. Density functional theory (DFT) calculations can provide insight into the atomic-scale reaction mechanisms helping to interpret a large amount of experimental data collected during decades. This presentation shows how DFT and bonding analysis can be used to describe the state of the surface during chemical reactions and the geometrical and electronic changes in both the surface and the adsorbated species. Our research has recently focused on the adsorption of hydrogen and acetylene on the intermetallic compound PdGa. Another example, where calculations match experiments, is the adsorption and dissociation of CO on Mo_2C. This carbide is poison resistant and presents an electronic structure similar to Pt metals. We analyze the charge re-arrangements after CO adsoption on a K doped surface, predict vibration frequencies and compare them with work function change and EELS data. Finally we will analyze the Se adsorption at different coverages on DO_3 FeSiAl(110) and the electronic structure of FeSiAl alloys and its relationship with soft magnetic properties. In our approach the models are built from experimental information in cooperation with the groups of Prof. M. Jenko (IMT) and Prof. Deck (Hungary).